The Role of Intermediate Structure and Level Fluctuations in Fission Cross Section Calculations

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Average Fission Cross Sections: Hauser-Feshbach Theory

The Hauser-Feshbach expression for average cross-sections in the compound nucleus theory. The full expression, appropriate for higher neutron energies, at which several orbital angular momenta may be significant, is

$$\sigma_{nr} = \frac{\pi}{k^2} \sum_J \frac{(2J+1)}{2(2I+1)} \sum_{s,s'=|I-i|}^{I+i} \sum_{l=|J-s|}^{J+s} \sum_{l'=|J-s'|}^{J+s'} \frac{T^J_{n(ls)} T^J_{r(l's')}}{T^J}$$

T_n is the transmission coefficient for the neutron entrance channel

T_r is the transmission coefficient for the exit channel

T^J is the sum of transmission coefficients over all channels available to the compound nucleus in a state of total angular momentum J.

Width fluctuations

The simple factorization contained in the Hauser-Feshbach formalism is not completely correct if the transmission coefficients are related to resonance properties as given above. The mixing of the independent particle states into the final compound states is stochastic in nature. Thus the reduced width amplitude for a given channel can be expected to have a gaussian distribution about a mean of zero. Translation of this into the frequency function for reduced widths leads to the Porter-Thomas distribution:

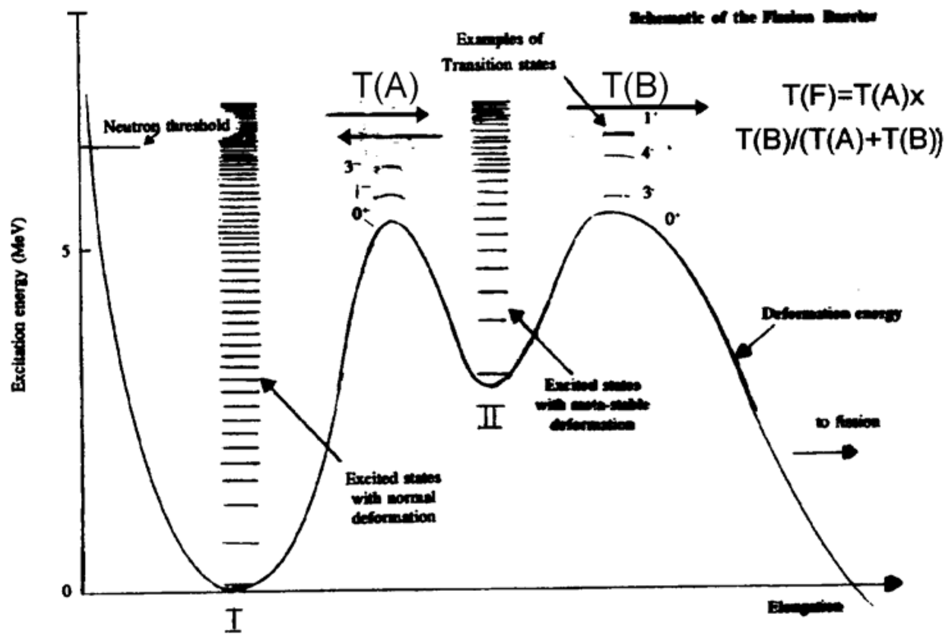
$$p(\gamma^2)\mathrm{d}\gamma^2 = \frac{1}{\sqrt{(2\pi\gamma^2\langle\gamma^2\rangle)}} \exp\left(-\frac{\gamma^2}{2\langle\gamma^2\rangle}\right)\mathrm{d}\gamma^2$$

This is a highly skewed frequency function that significantly affects averaging over the mean cross-section across a single resonance level in obtaining the cross-section over many resonances. An effective averaging factor $\mathbf{S_{nr}}$ is inserted into the Hauser-Feshbach formula to allow for this. Its effect on an elastic scattering cross-section is to <u>increase</u> it by up to a factor of 3.

The important reaction cross-sections are generally <u>decreased</u>. The averaging factor can be as low as 0.7 for normal particle and radiative capture cross-sections.

The Fission Reaction

Fission is more complicated than a simple particle reaction. At relatively low excitation energies only one or a few major saddle-point channels are open, each with width fluctuations characteristic of the Porter-Thomas distribution. But fission of the actinides is governed by the double-humped barrier.



Statistical Model: transmission coefficients $\boldsymbol{T}_{\mathbf{A}}$ and $\boldsymbol{T}_{\mathbf{B}}$ for separate barrier peaks together give the fission coefficient $\boldsymbol{T}_{\mathbf{F}}$ for use in Hauser-Feshbach theory expression for average cross-sections in the compound nucleus theory. This model ignores intermediate structure.
Transmission factors for the separate inner and outer barriers are denoted by T_A , T_B respectively. The statistical expression for the transmission factor for penetration of the whole barrier is:

$$T_F \approx T_A \, T_B/(\, T_A + T_B)$$

This is the transmission coefficient to employ for fission cross-sections in the Hauser-Feshbach formula.

AVERAGE FISSION CROSS SECTIONS:
The role of intermediate structure and level fluctuations
in the near-barrier energy region

Intermediate structure in the cross-section is an important consequence of the double-humped fission barrier and must be taken into account when calculating average fission cross-sections at sub-barrier energies. Averaging over intermediate resonance structure due to class-II levels gives a different formula from Hauser-Feshbach: for neutron-induced fission it is:

$$\sigma_{nf} = \pi ƛ^2 g_J \frac{T_n}{\{1 + (T_I/T_F)^2 + (2T_I/T_F)\coth[\_(T_A + T_B)]\}^{1/2}}$$

where T_n is the entrance neutron channel transmission coefficient and T_I is the sum of particle emission and radiation coefficients for class-I states.

Note: a uniform picket-fence model is assumed for both class-I and class-II states (partial widths and spacings do not deviate from average values)

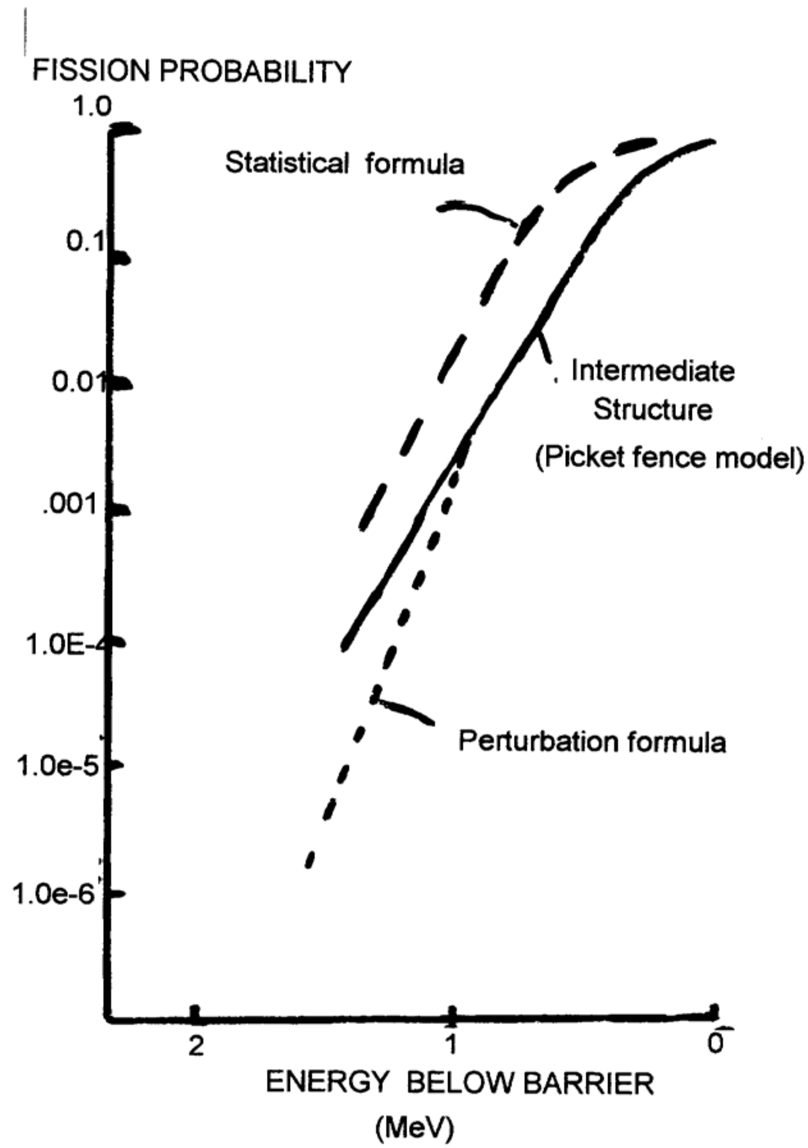
The fission probability (for given J^π)

$$P_F = \sigma_{nf} / \pi ƛ^2 g_J T_n$$

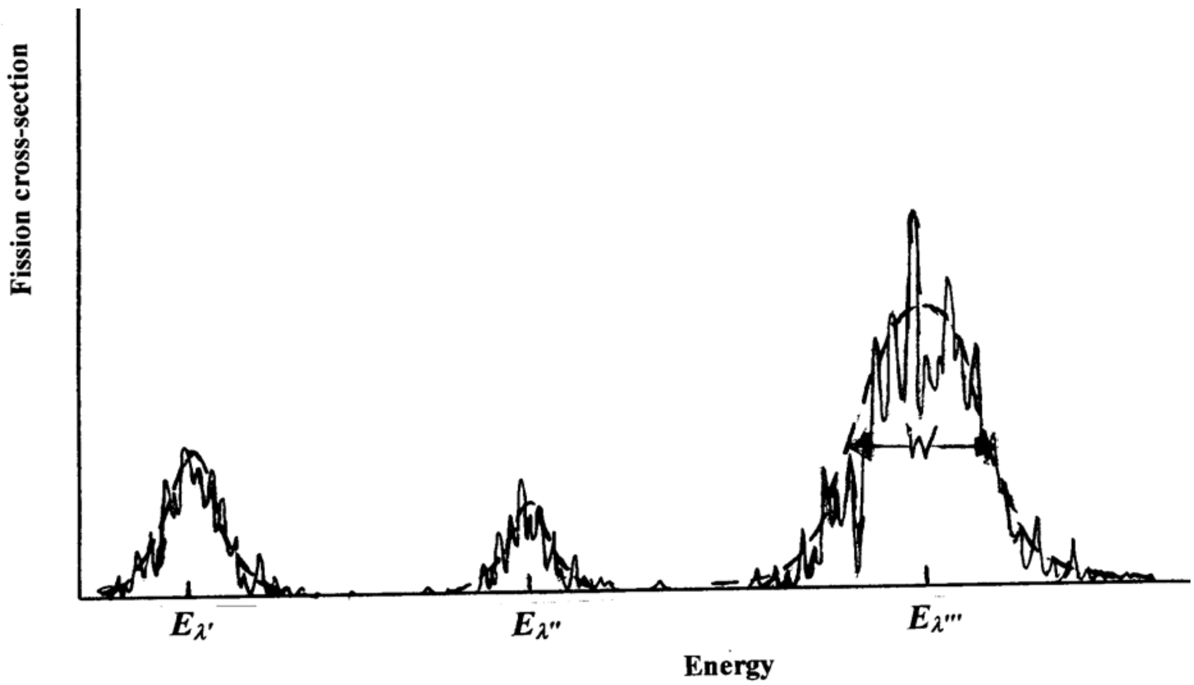
is shown in next Figure for inner and outer barriers of equal height, and widths $\hbar\omega_A$ = 1.0MeV, $\hbar\omega_B$ = 0.6MeV, in comparison with the statistical model fission probability,

$$T_F / (T_F + T_I).$$

Illustration of difference between Statistical (Hauser-Feshbach) model and intermediate structure formula for sub-barrier fission probability, P_F , with competition only between capture and fission



Level fluctuations



Width of intermediate resonance:

$$2W_{\lambda\mathrm{II}} \approx \Gamma_{\lambda\mathrm{II(F)}} + \Gamma_{\lambda\mathrm{II(C)}}$$

Strength of intermediate resonance:

$$\propto \Gamma_{\lambda\mathrm{II(F)}}\, \Gamma_{\lambda\mathrm{II(F)}} / W_{\lambda\mathrm{II}}$$

Relations for the coupling width:

$$\langle \Gamma_{\lambda\mathrm{II(C)}} \rangle = D_{\mathrm{II}} T_A / 2\pi\,, \qquad \Gamma_{\lambda\mathrm{II(C)}} = 2\pi \langle H(\lambda_{\mathrm{II}}, \lambda_{\mathrm{I}})^2 \rangle_{\lambda\mathrm{I}} / D_{\mathrm{I}}$$

Fission width of fine structure resonance:

$$\Gamma_{\lambda\mathrm{(F)}} \propto H(\lambda_{\mathrm{II}}, \lambda_{\mathrm{I}})^2\, \Gamma_{\lambda\mathrm{II(F)}} / [(E_{\lambda\mathrm{II}} - E)^2 + W_{\lambda\mathrm{II}}{}^2]$$

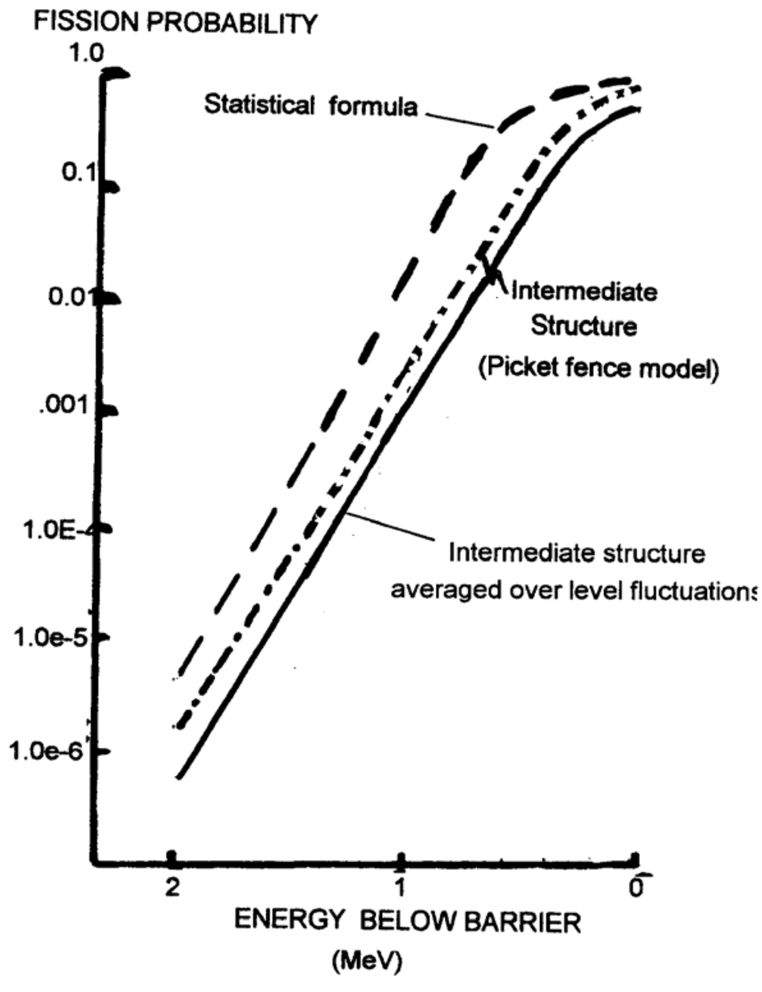
Strength of fine structure resonance:

$$\propto \Gamma_{\lambda\mathrm{(n)}}\, \Gamma_{\lambda\mathrm{(F)}} / \Gamma_{\lambda}^2$$

Porter-Thomas type distributions apply not only to reduced neutron widths of class-I (fine-structure) levels, but also to coupling and fission widths of class-II levels, and to class-I to class-II squared coupling matrix elements. These have an important effect on the average fission cross-section.

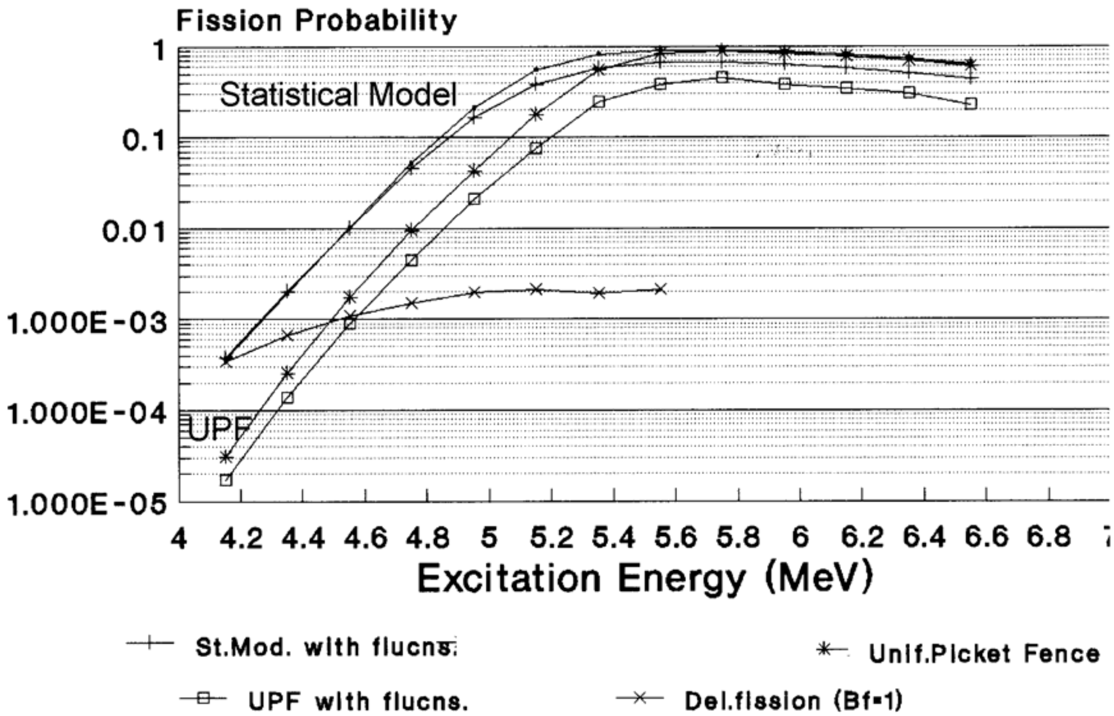
Calculations of averages are made by Monte Carlo procedures involving pseudo-random selection of level parameters and coupling matrix elements, and diagonalisation to obtain final resonance parameters for final cross-section calculation.

Example: sub-barrier fission probability (fission-capture competition only)



Note: analysis of P_F (for example, from *d,pf, t,pf* etc. reactions) to obtain barrier height information is strongly affected (up to 0.4 MeV in above example) by inclusion of intermediate structure <u>and</u> all level fluctuations.

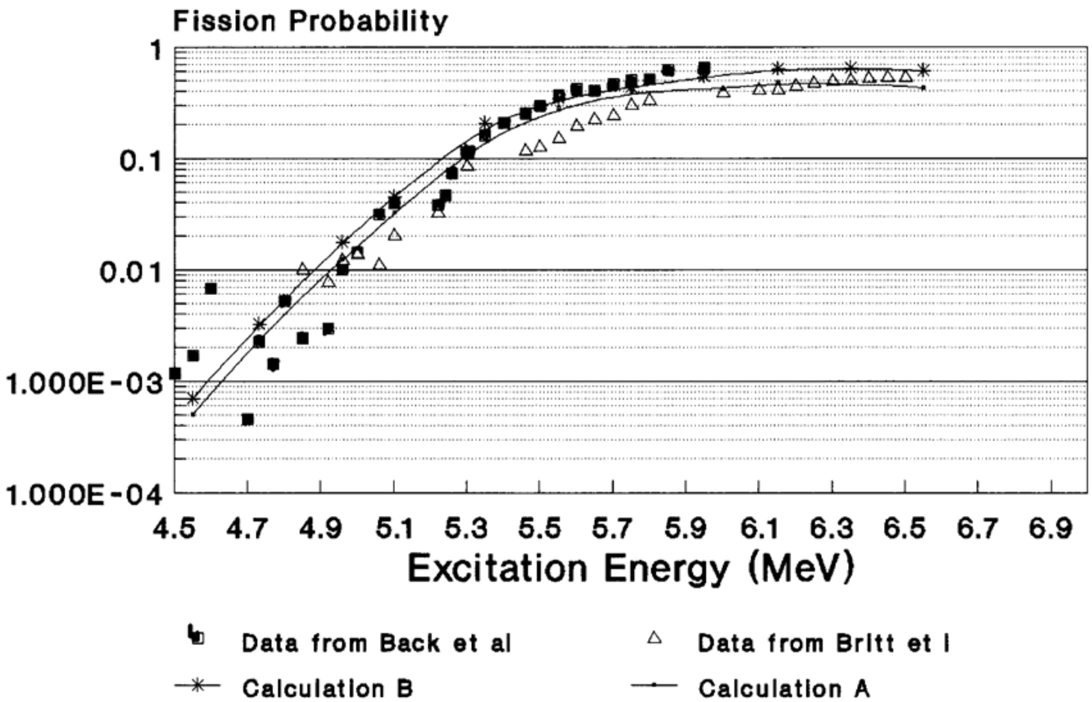
More detailed study of (t,pf) reaction:
The *(t,p)* reaction, acting on an even target, populates even spin, even parity and odd-spin, odd-parity states in the compound nucleus



Model for $J^{\pi} = 4^{+}$ states populated in (t,pf):

Barriers at 5.5 MeV (for 0^{+}), 4^{+} transition state 0.07 MeV above barriers.
$h\omega_A = 1.0$ MeV, $h\omega_B = 0.6$ MeV

Inclusion of 3$^-$ states with barrier A states at 0.5 (m.a.), 0.7 (b), 0.56 (γ+ma), 0.76 ((γ+b) MeV and barrier B states at 0.1 (ma), 0.6 (b), 0.9 (γ+ma), 0.7 (ma+b) MeV.



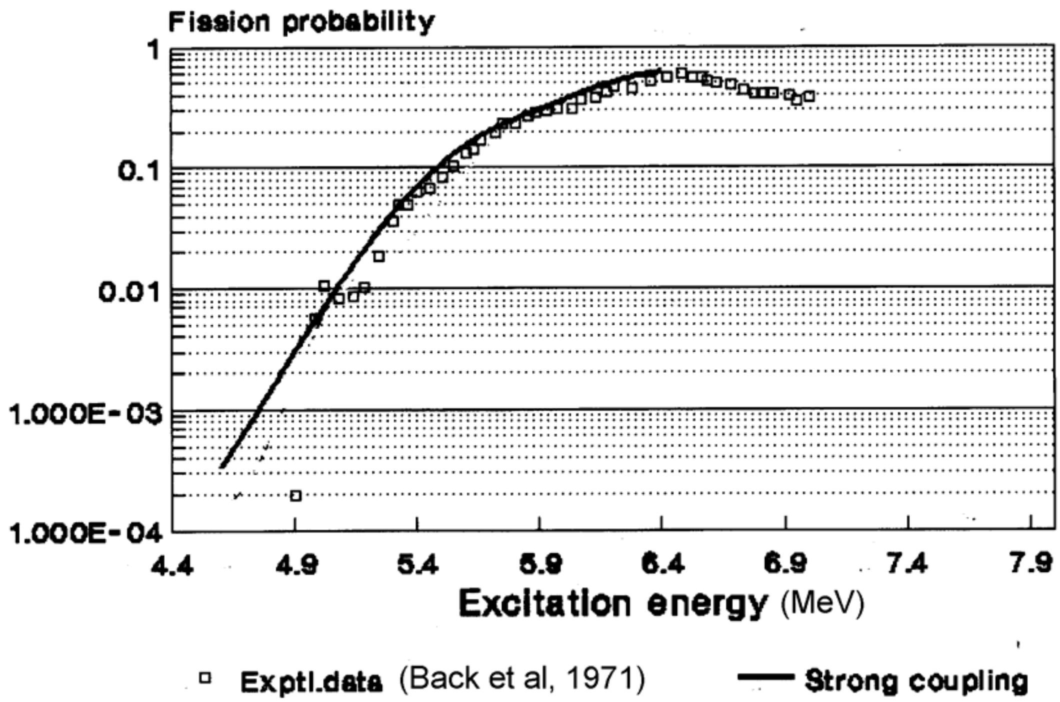
Calculation A is for simple 1-channel 4$^+$ model averaged with 3- .

Calculation B is for 3- averaged with following 4+ model:
Barrier A states: 0.07 ("gd"+rotn.), 0.12 (γ), 0.20(2γ) MeV
Barrier B states: 0.05 ("gd"+rotn.), 0.8 (γ), 0.70 (ma+b) MeV

Data for ^{234}U(*t,pf*) are from Britt, Rickey and Hall (1968) and Back, Hansen, Britt and Garrett (1974)

Application to U-235 (d,pf) - full calculation

Data are from Back, Bondorf, Ostroschenko, Pedersen and Rasmussen (1971)

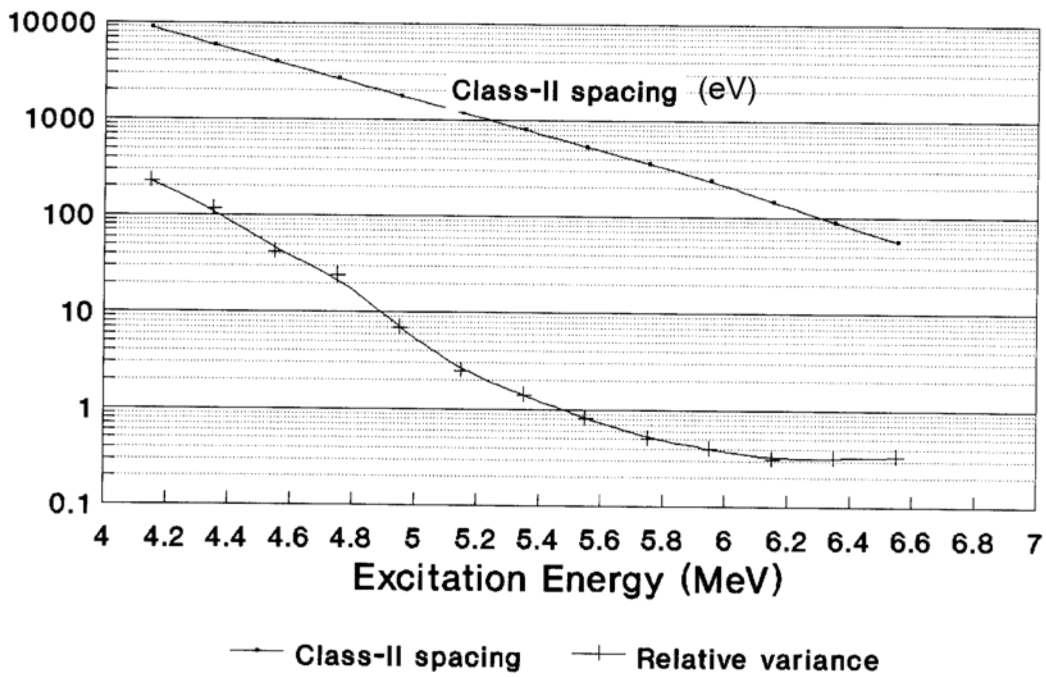


U-235 (d,pf)

Fluctuations in "local" average cross-sections

"Local" average fission cross-section is defined as the average of the cross-section over a single class-II spacing.

The graph below shows the relative variance (variance/square of mean) for the 3- levels in the above model as a function of excitation energy.



Class-II spacing & cross-sectn.variance

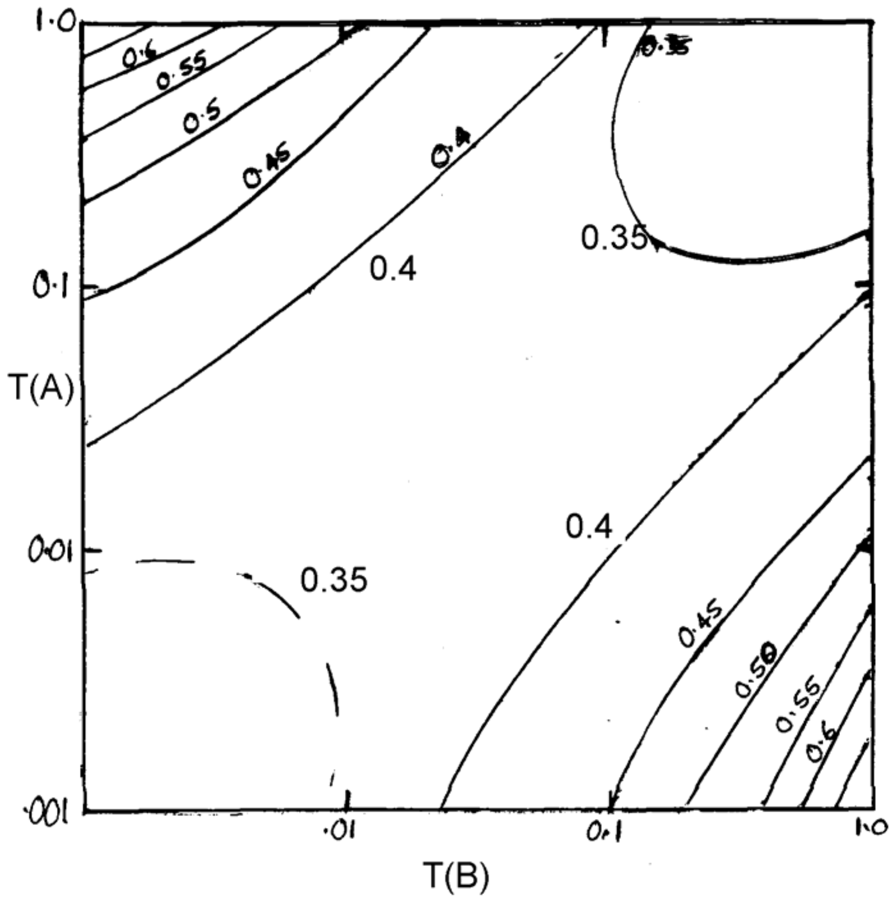
Note extremely high relative variance at low excitation energies. This is largely due to accidental near-degeneracy between class-I and class-II levels when class-II coupling and fission widths are less than the class-I level spacing. This gives rise to questions about interpretation of "vibrational resonances".

Application to Neutron Cross-sections

As in Hauser-Feshbach we employ the convention of an averaging factor S, but in this case applied to the average cross-section from the intermediate structure uniform picket fence model:

$$<\sigma_F> = \sigma_{UPF}\, S_{nf}$$

Below is a contour diagram of S_{nf} in the plane of $\boldsymbol{T_A}$ and $\boldsymbol{T_B}$ (1 saddle-point channel) for neutron energy 10 keV.



$\boldsymbol{S}$ has a very significant effect in reducing the fission cross-section in channels that are only partially open. For example: the s-wave cross-section of the isomer of U-235 ($I^\pi = 1/2^+$), in which the compound nucleus excitation energy is lower than the saddle-point energy of the $J^\pi = 1^+$ state - the net effect is to give a fission cross-section at low neutron energies that is about one half of that of the ground state ($I^\pi = 7/2^-$)

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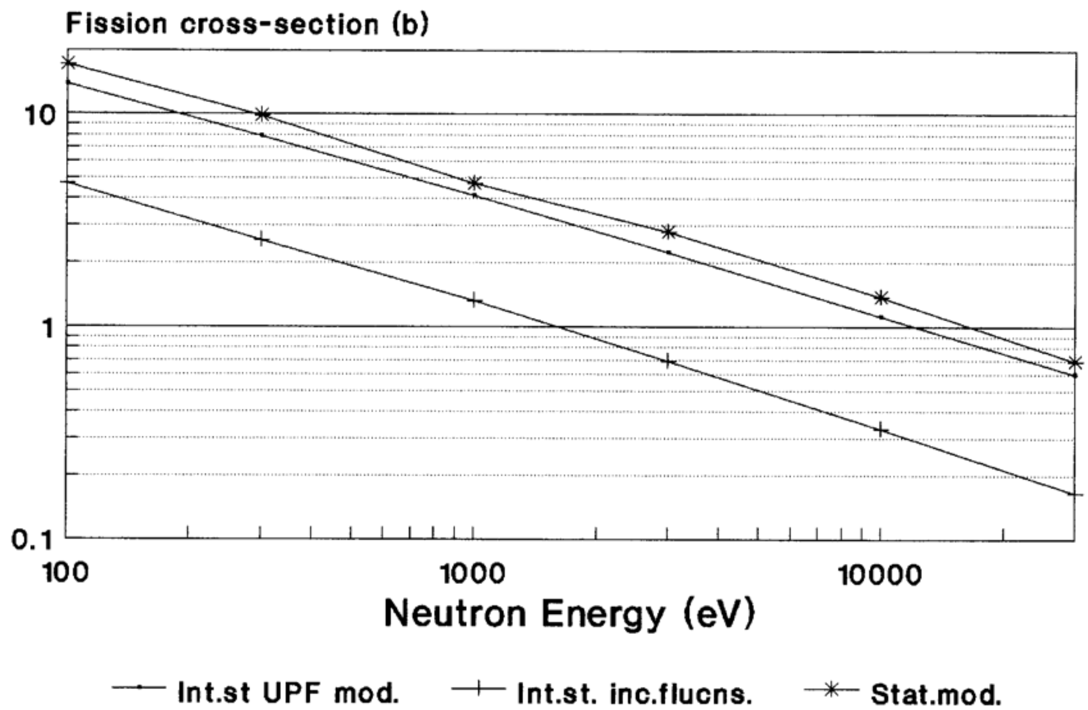
Barriers in Compound Nucleus U-236 assumed to be at 5.5MeV (for 0+)
(neutron separation energy is 6.55 MeV)

Barrier A: ma vibn. at 0.5 MeV, b vibn. at 0.8 MeV ∴ combn.1+ at 1.3 MeV

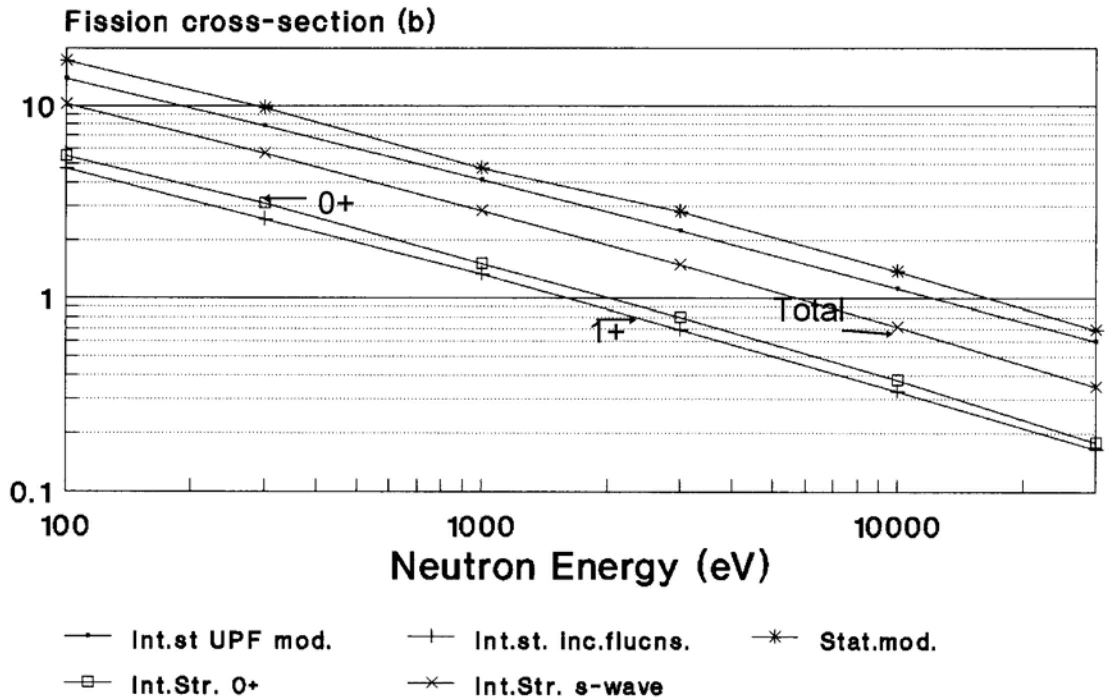
Barrier B: ma vibn. at 0.1 MeV, b vibn. at 0.7 MeV ∴ combn. 1+ at 0.8 MeV

1+ cross-sections:



U-236(n,f) 1+

1+, 0+ and total s-wave fission cross-section of U-235m ($I^{\pi} = 1/2^{+}$)



Conclusions

1) Fission is treated in Hauser-Feshbach theory by using a transmission coefficient that is based on the assumption that there is gross damping in the secondary well, but ignores the quasi-discrete level structure.

2) Intermediate structure due to class-II levels in the second well has a large reduction effect on the average fission probability near and below the barrier; the cross-section expression is different from Hauser-Feshbach but approaches it asymptotically.

3) Porter-Thomas and Wigner type fluctuations in both class-I and class-II level parameters <u>and</u> the coupling matrix elements also have a large reduction effect on the average fission cross-section.

4) Interpretation of fission barrier heights from data (such as *t,pf*) can be changed by 0.3 to 0.4 MeV by inclusion of above effects.

5) Intermediate structure and its fluctuations contribute to the expected reduction of the ^{235m}U isomer fission cross-section below that of the ground state.